Isopropyl ether

108-20-3 | DTXSID4021890

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 8.93 days

Global applicability domain: Outside

Local applicability domain index: 3.83e-01

Confidence level: 8.23e-01

Nearest Neighbors from the Training Set

Image not found
2,2-Dimethylbutane
Measured: 880
Predicted: 16.2

Image not found
Pentane
Measured: 40.7
Predicted: 6.52

Image not found
Pentane,3,3-dimethyl-
Measured: 157
Predicted: 11.9

Image not found
n-Hexane
Measured: 157
Predicted: 7.45

Image not found
Heptane
Measured: 88.3
Predicted: 7.54